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A Sensitivity Analysis of the Gas Dynamics Equations

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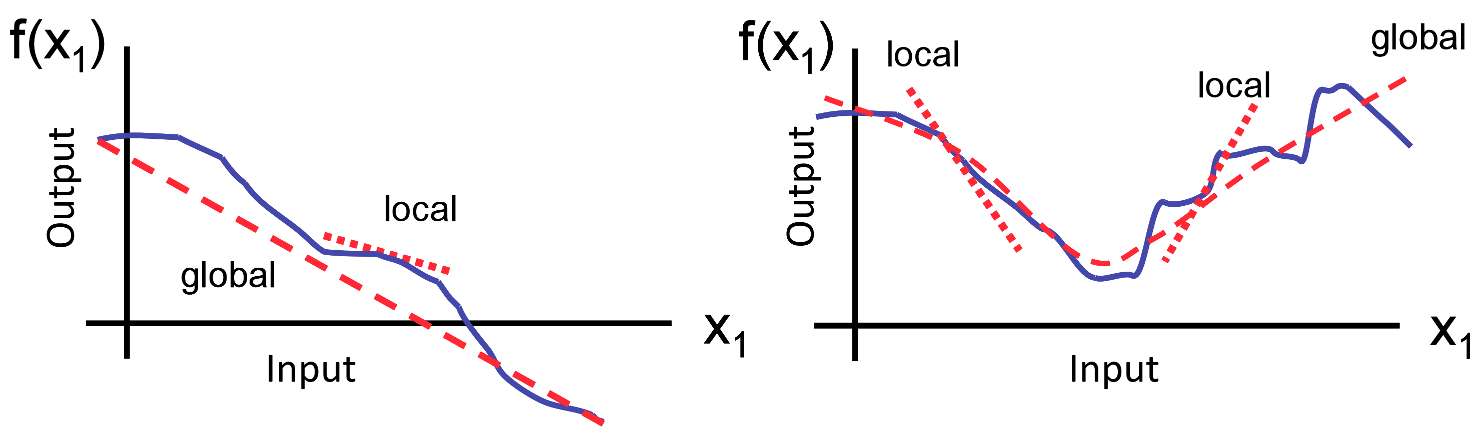
What is Sensitivity Analysis?

- Sensitivity Analysis (SA) is a way to order the input variables to a model according to their relative importance to the model's output.
- The results of SA can be used to inform us about:
  - Optimization
  - Uncertainty Quantification
  - Which inputs to gather more data on
  - How to better control an experiment
- Local SA: local linear or under-resolved behavior can be misleading.
- Global SA: can be computationally expensive (use meta-modeling).



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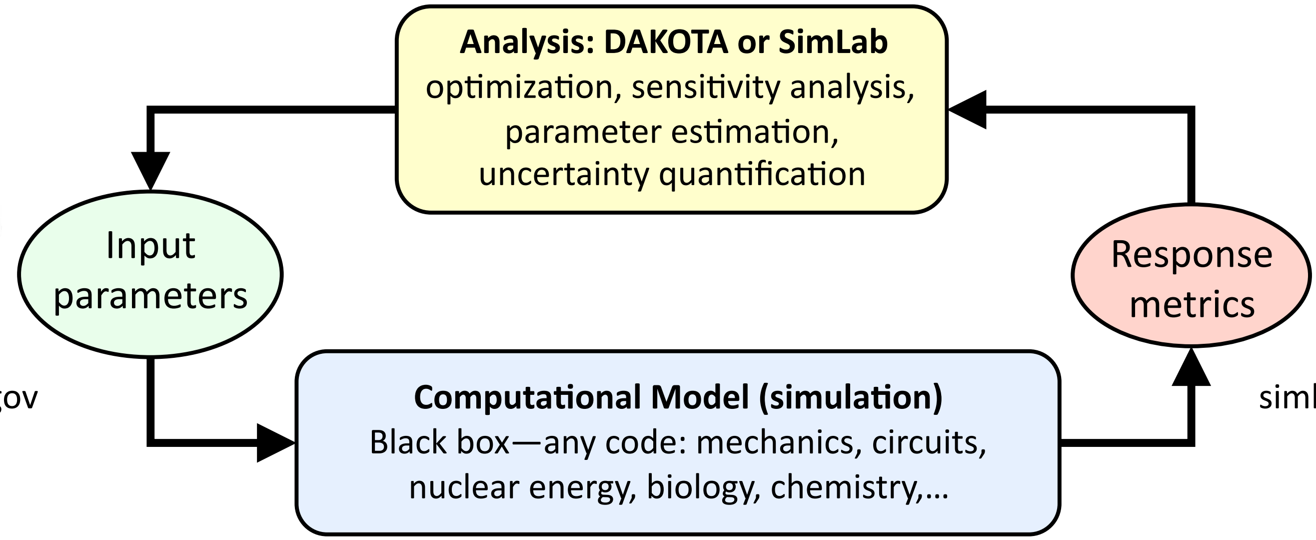
We conduct sensitivity analyses with DAKOTA and SimLab.



dakota.sandia.gov

simlab.jrc.ec.europa.eu

- DAKOTA has a generic interface to simulation software, contains advanced methods, and can automate "parameter variation" studies, including:
  - Sampling (LHS, quasi-MC, classical experimental designs)
  - Dempster-Shafer evidence theory
  - Stochastic expansion methods: Polynomial chaos, stochastic collocation
  - Nested approaches for quantifying epistemic and aleatory uncertainties
- SimLab is a development framework designed for Monte Carlo-based uncertainty and sensitivity analysis.

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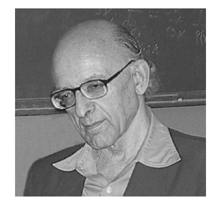
Correlation and Variance-Based Decomposition (VBD) characterize the global sensitivity of model outputs Y to model inputs X.

- Goal: to assess outputs for a specified range of inputs.
- Correlation analysis identifies the strength and direction of a *linear* relationship between input and output.
- VBD identifies the fraction of the variance in the output that can be attributed to an individual variable alone or with interaction effects.
  - Main effect sensitivity S_i is the fraction of the uncertainty in Y that is due to input X_i *alone*

$$S_i = \frac{\mathrm{Var}_{X_i}\left[E(Y|X_i)\right]}{\mathrm{Var}(Y)}$$

  - Total effect index T_i is the fraction of the uncertainty in Y that is due to X_i *and its interactions with other variables*

$$T_i = \frac{E\left[\mathrm{Var}(Y|X_{-i})\right]}{\mathrm{Var}(Y)}$$



I.M. Sobol' developed these ideas

  - Calculation of S_i and T_i requires the evaluation of m-dimensional integrals, approximated by Monte-Carlo sampling.

$$X_{-i} \equiv (X_1,\ldots,X_{i-1},X_{i+1},\ldots,X_m)$$

  - The evaluation of these quantities is *computationally intensive*, as replicated sets of samples are evaluated.

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Meta-models provide an alternative to sampling-based VBD.

- Build the meta-model using some of the data.
  - This is reasonable for moderately high dimensional data
- Estimate the sensitivity indices using the meta-model.
  - This can be done (i) with the same data used to construct the meta-model or (ii) with data that was *not* used to construct the meta-model
- Meta-models can be used to generate confidence intervals of the computed indices.
  - These confidence intervals give a measure of the “variability” or “uncertainty” in the computed indices.
- There are several different ways to construct the meta-models.
  - “Regression surfaces” (regression and smoothing)
  - Stochastic expansions (polynomial chaos, stochastic collocation)

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Regression surface models are alternatives to sampling-based approaches.

- SDP = State-Dependent Parameter Regression
  - SDP modeling* is a class of non-parametric smoothing, first suggested by Young§, that is similar to smoothing splines and kernel regression approaches but is performed using recursive (non-numerical) Kalman filter and associated fixed interval smoothing.
  - SDP is good for additive models and can adapt to local discontinuities, strong non-linearity, and heteroskedasticity in the response.
- ACOSSO = Adaptive COmponent Selection and Smoothing Operator
  - ACOSSO† is a multivariate smoothing-spline approach (COSSO‡) that is augmented by a weighted (w_j), scaled (λ) penalty function:

$$\hat{f} = \min_{f \in \mathcal{F}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \left(Y_i - f(x_i) \right)^2 + \lambda \sum_{d=1}^{\overbrace{D}^{D\,=\,\#\text{ inputs}}} w_d \left\| P^d f \right\| \right\}$$

  - ACOSSO is thought to perform best for a reasonably smooth underlying response.
- DACE = Design and Analysis of Computer Experiments
  - Gaussian Process emulator for the output responses.

§ Young, P. C. “The identification and estimation of nonlinear stochastic systems,” in *Nonlinear Dynamics and Statistics*, A. I. Mees et al., eds., Birkhauser, Boston (2001).

* Ratto, M., Pagano, A., Young, P. C., “State dependent parameter meta-modelling and sensitivity analysis,” *Comput. Phys. Comm.,* **177**, pp. 863–876 (2007).

† Storlie, C.B., Bondell, H.D., Reich, B.J., Zhang, H.H., “Surface estimation, variable selection, and the nonparametric oracle property,” *Stat. Sinica,* to appear (2010).

‡ Y. Lin,Y., and H. Zhang, H., “Component selection and smoothing in smoothing spline analysis of variance models,” Ann. Stat., **34**, pp. 2272–2297 (2006).

Stochastic Expansion Methods provide another alternative to sampling-based VBD.

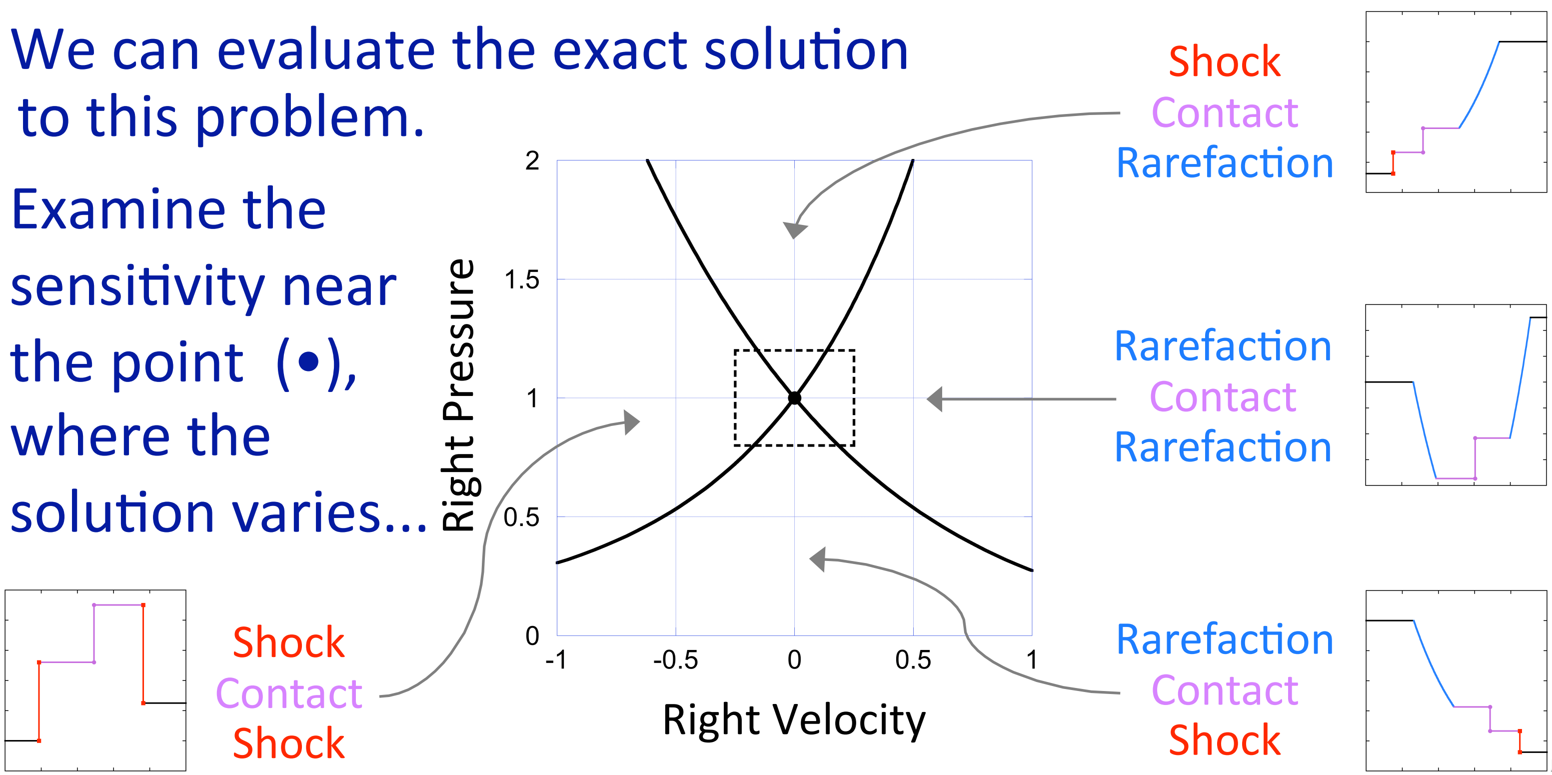
- Stochastic expansion methods — Polynomial Chaos Expansion (PCE) or Stochastic Collocation (SC) — produce functional representations of stochastic variability.
- Sudret* (i) demonstrated that the sensitivity indices are explicit functions of the stochastic expansion, and (ii) derived the PCE case.
  - Once the PCE is obtained, sensitivity indices are calculated *explicitly*, i.e., without additional sampling
- Tang§ derived the sensitivity indices as analytic functions of SC.
- Both of these techniques have been implemented in DAKOTA.
- This approach can be *very efficient*, since the calculation of sensitivity indices does *not* require additional function evaluations.

* Sudret, B., “Global Sensitivity analysis using polynomial chaos expansion,” *Rel. Engr. & Syst. Safety*, **93**, pp. 964–979 (2008).

§ Tang, G., Iaccarino, G., Eldred, M.S., "Global Sensitivity Analysis for Stochastic Collocation Expansion," paper AIAA-2010-2922 in *Proceedings of the 12th AIAA Non-Deterministic Approaches Conference*, Orlando, FL, 12–15 April 2010.

We consider Sensitivity Analysis of a shock tube problem.

- Initial state: $(\rho, p, u, \gamma) = \begin{cases} (1.0,\ 1.0,\ 0.0, 1.4), & 0 \le x < 0.5 \quad \text{“Left”} \\ (0.125, 1.0, 0.0, 1.4), & 0.5 < x \le 1.0 \quad \text{“Right”} \end{cases}$
- Fix the left state; vary the right state; consider fixed $t_{\text{final}} = 0.2$
- We can evaluate the exact solution to this problem.
- Examine the sensitivity near the point (•), where the solution varies...



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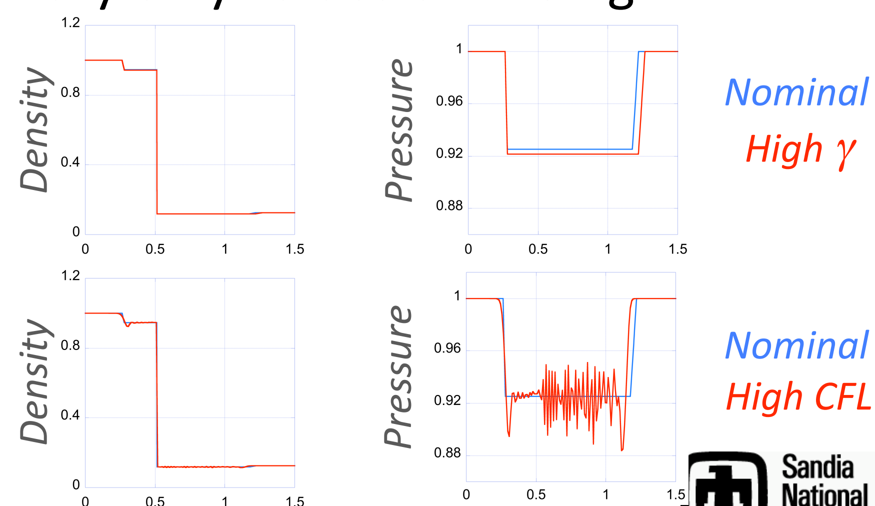
We fix the final time and the left state, but vary both the right state and a numerical parameter.

		Input	*Why?*
Right	X_1	Initial pressure on right	Uncertainty in initial condition
Right	X_2	Initial velocity on right	Uncertainty in initial condition
Right	X_3	Polytropic index γ on right	Uncertainty in material model
	X_4	CFL parameter: $c_s\,\Delta t/\Delta x$	Numerical parameter

- From the self-similar nature of the solution, only one state need be varied, not both: therefore, we vary only values on the right.

- Higher pressure, higher γ $\rightarrow$ higher sound speeds and faster wave propagation

- 0 < CFL < 1 $\rightarrow$ stable
  CFL > 1 $\rightarrow$ unstable

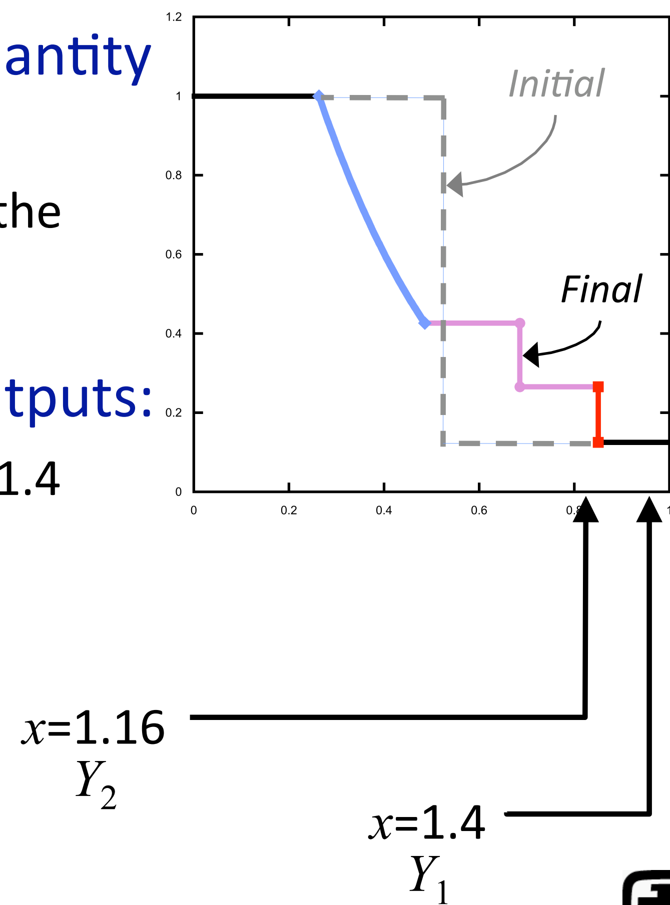


The outputs are values at fixed locations.

- These outputs correspond to a experimental diagnostics.

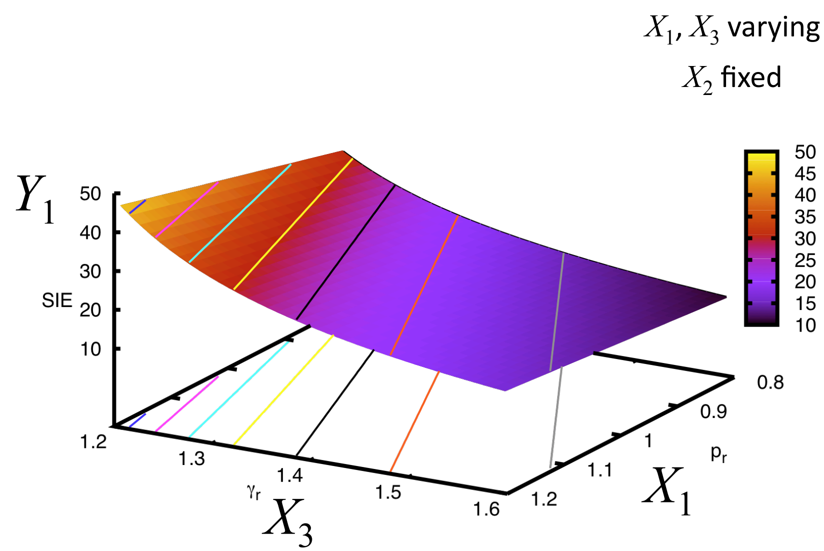
- These outputs measure some quantity at a specific location.
  - We record the value at the end of the simulations, t=0.2

- In this study, we examine two outputs:
  - Y_1 = specific internal energy at x = 1.4
  - Y_2 = density at x = 1.16



We can evaluate the <u>exact</u> solution for all outputs, e.g., Y_1, which is the SIE at $x = 1.4$.

- Y_1 is a simple output that we use as a test.
- No waves reach this location, so the SIE does not change from at initial value.
  - This value is a function of X_1 and X_3 only.
  - Sensitivity indices should show this dependence.

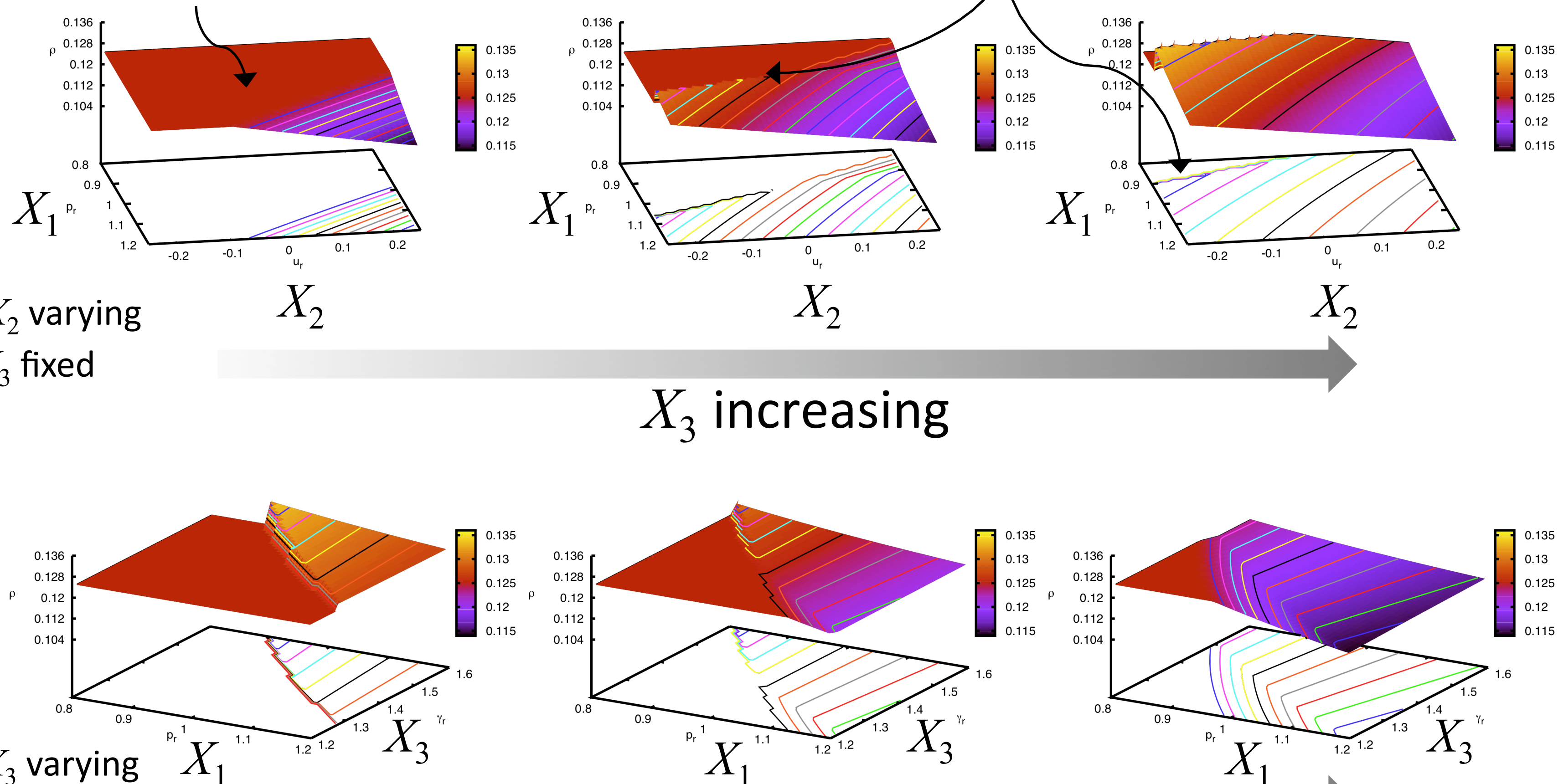


Output surface slice for the <u>exact</u> solution

The exact response surface for Y_2, the density at x = 1.16, is quite different.

Flat regions mean that no waves have reached here

Sharp “cliffs” mean shocks



X_1, X_2 varying
X_3 fixed

X_3 increasing

X_1, X_3 varying
X_2 fixed

X_2 increasing

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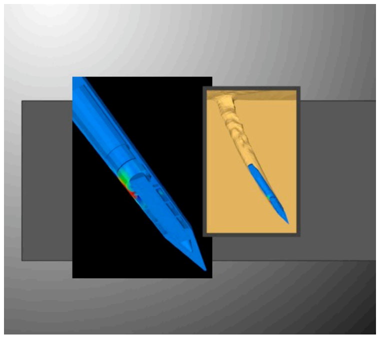
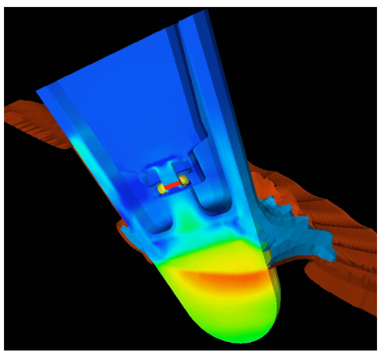
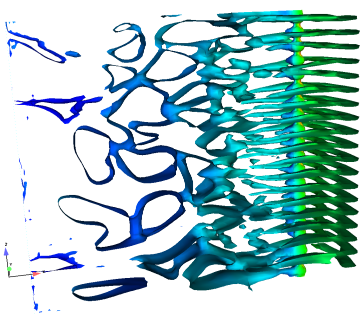
We simulate this problem with the ALEGRA multi-physics code.

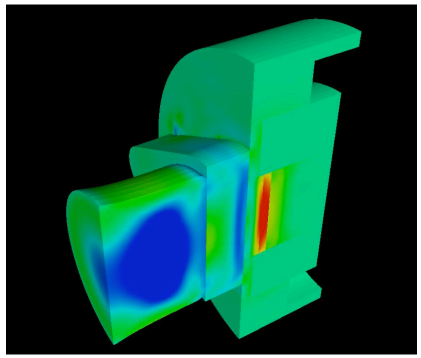
Shock and Multi-physics

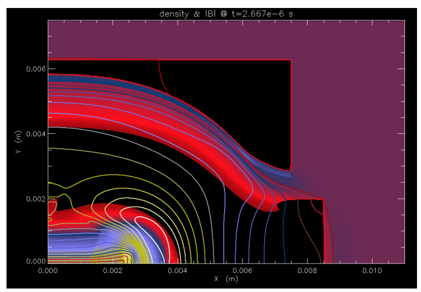


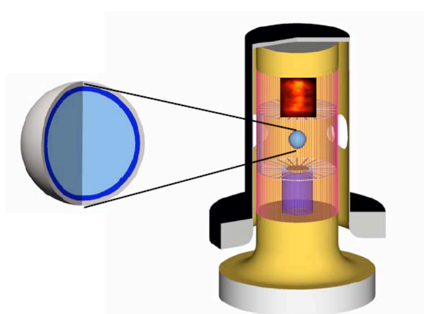




HEDP Theory and ICF Target Design





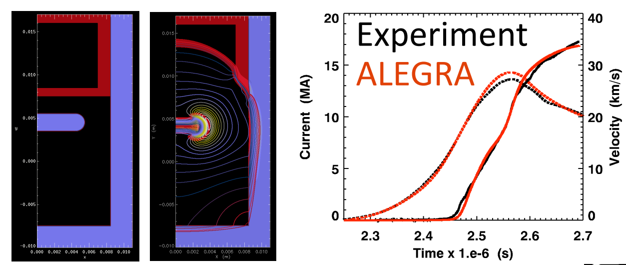


Overview

- The ALEGRA suite of applications models shock and high energy environments for solids, fluids, and plasmas using a multi-material arbitrary Lagrangian-Eulerian (ALE) multi-physics methodology.
- ALEGRA applications run on large, parallel, message-passing architectures in 2-D and 3-D geometries.

ALEGRA Applications

- Armor Design and Analysis
- Shaped Charges & Explosively Formed Penetrators
- Railgun Design and Analysis
- Magnetohydrodynamics (MHD)
- Z-pinch, Inertial Confinement Fusion
- Isentropic Compression Experiments/Magnetic Flyers



Isentropic Compression: Magnetic Flyer Prediction vs. Expt

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The underlying equations in ALEGRA are related to hyperbolic conservation laws.

- The fundamental equations are statements of conservation laws:

$$\frac{\partial \underbrace{\boxed{U}}_{\text{State}}}{\partial t} + \operatorname{div} \underbrace{\boxed{f(U)}}_{\text{Flux function}} = \underbrace{\boxed{S(U)}}_{\text{Source term}} \qquad x \in \Omega \subset \Re^3,\ t \geq 0$$

  - Depending on the physics modeled, the state U may include, e.g.:
    - Internal state variables from material strength models
    - Magnetic field quantities for MHD simulations
  - These are discretized on a hexahedral mesh in the Arbitrary Lagrangian-Eulerian framework, amenable to general meshing and remapping.
- The gas dynamics equations are the "simplest" nonlinear physics equations that form a basic part of the full set of models in ALEGRA.
- This study is a prototype for the future analysis of problems with more complicated physics.

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The simulation response for Y_2, the density at x = 1.16, is different from the exact response.

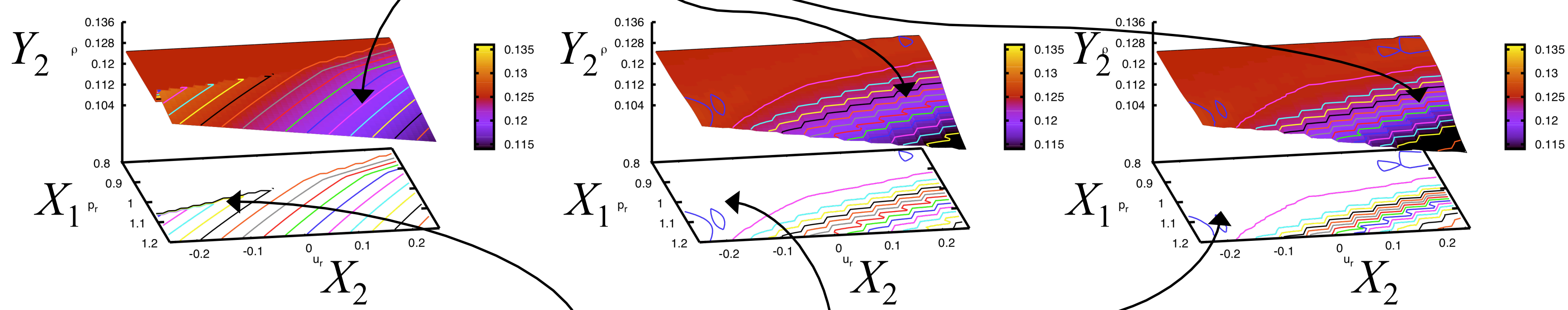
Surface is nosier —the noise increases with X_4 , the CFL parameter.

X_1, X_2 varying
X_3, X_4 fixed

Exact

Simulation

Simulation



X_4 = 0.805

X_4= 1.195

The shocks in the simulation are not as sharp as the exact shocks

- For this problem, most simulation response surfaces differ only slightly from the exact response surfaces.

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We show results for estimators of the main (S) and total (T) sensitivity indices for several methods.

Meta-models
- DACE 256 Gaussian process approach, 256 samples
- ACOSSO 256 adaptive smoothing spline, 256 samples
- SDP 256 non-parametric smoothing, 256 samples

Analytic VBD
- PCE6 1296 analytic VBD, 6th-order, uniform distr., 1296 samples
- JRC 196k 196k sample, Sobol´/Saltelli estimates — *The usual "gold standard"*
- PCE4 256 analytic VBD, 4th-order, uniform distr., 256 samples

LHS Sampling
- LHS 60000 6.e+4 samples, Latin Hypercube Sampling VBD
- LHS 6000 6.e+3 samples, Latin Hypercube Sampling VBD

Full Factorial
- A-EXACT 160k 1.60e+5 (=20^4) ALEGRA, "full factorial" VBD
- A-EXACT 2.56M 2.56e+6 (=40^4) ALEGRA, "full factorial" VBD
- R-EXACT 160k 1.60e+5 Riemann (exact), "full factorial" VBD
- R-EXACT-2.56M 2.56e+6 Riemann (exact), "full factorial" VBD

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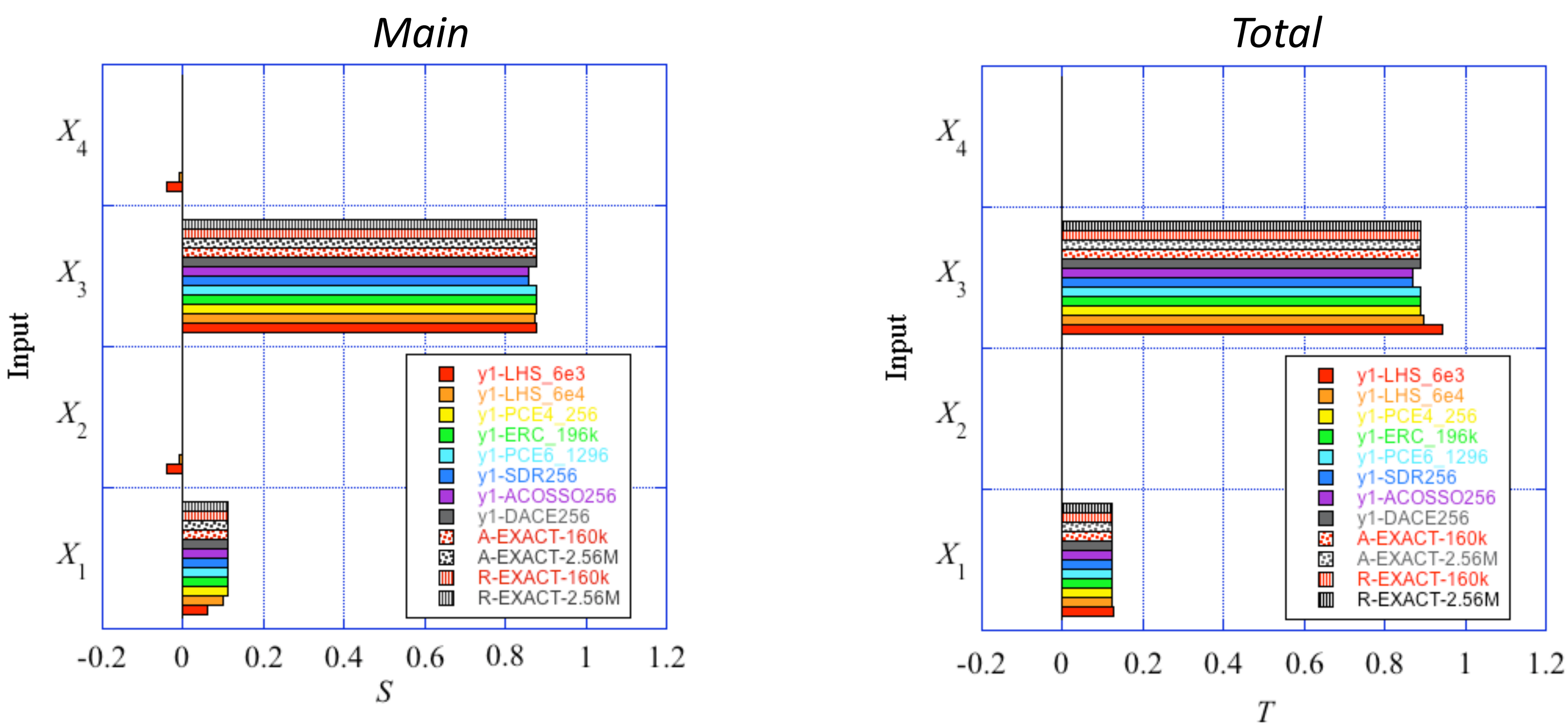
The sensitivity indices S and T for Y_1 perform similarly for all approaches.

- As anticipated, Y_1 (SIE) depends strongly on X_1 (p_R) and X_3 (γ_R)
- Sampling, meta-model, and "exact" results are all consistent.

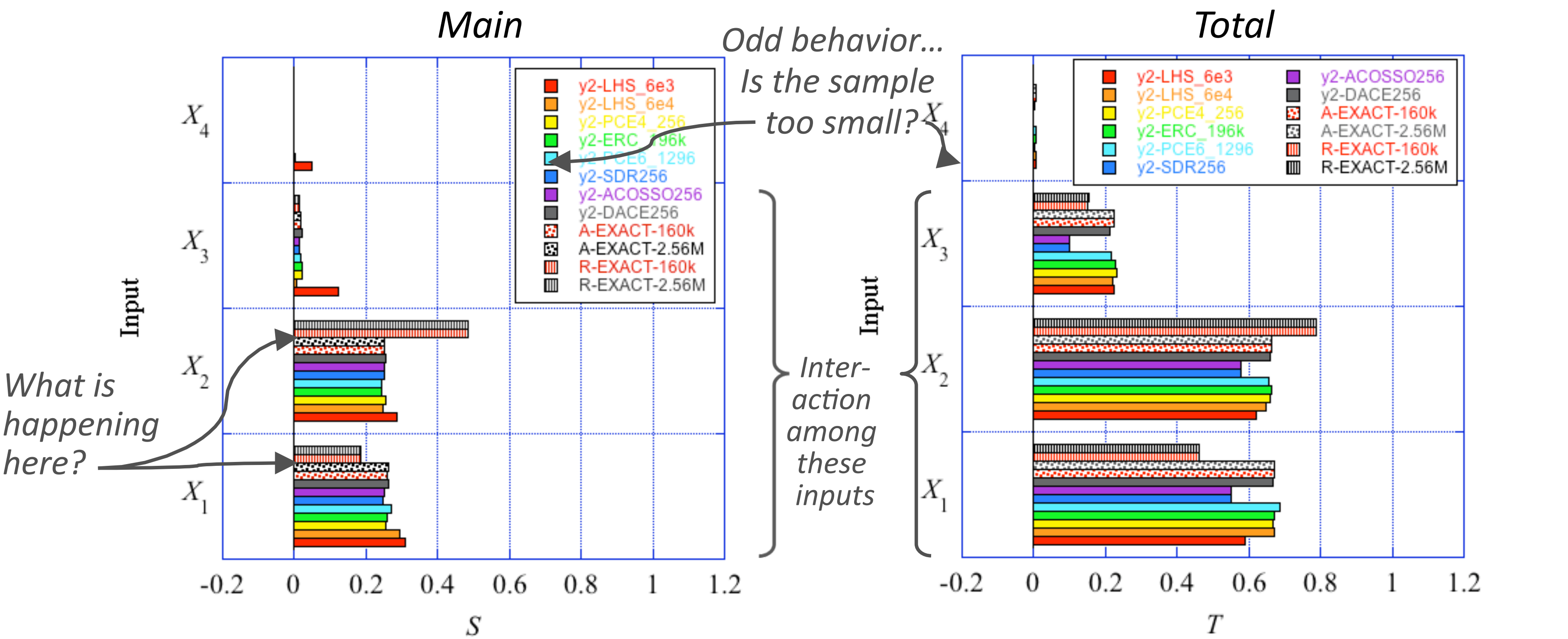


LHS 6000 PCE4 256 PCE6 1296 ACOSSO 256 A-EXACT 160k R-EXACT 160k

LHS 60000 JRC 196k SDP 256 DACE 256 A-EXACT-2.56M R-EXACT-2.56M

The sensitivity indices for Y_2 have some unusual features.

- For Y_2 (final right ρ), LHS has different ranking, particularly for 6.e+3 samples and esp. wrt X_3 (γ_R) and X_4 (CFL).

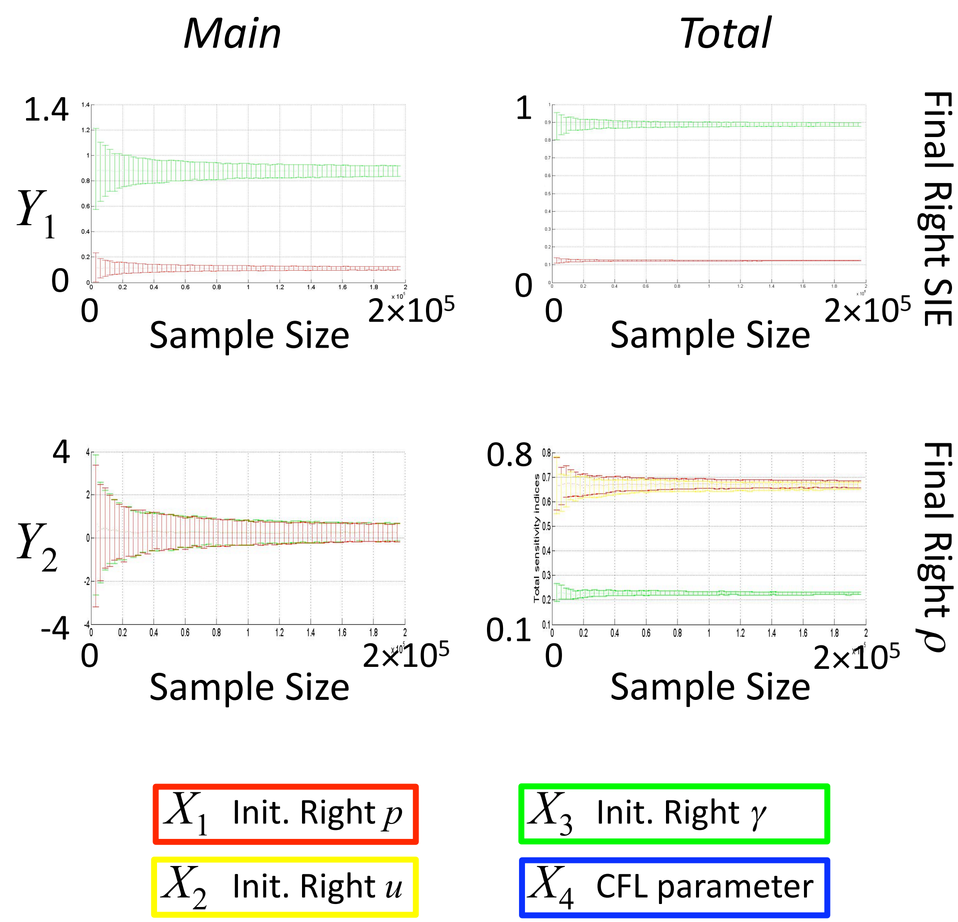


LHS 6000 | PCE4 256 | PCE6 1296 | ACOSSO 256 | A-EXACT 160k | R-EXACT 160k

LHS 60000 | JRC 196k | SDP 256 | DACE 256 | A-EXACT-2.56M | R-EXACT-2.56M

Estimators of the main and total sensitivity indices§ converge under quasi-random sampling.

- Confidence intervals were calculated with a bootstrap technique.*
- Confidence intervals *decrease* with increasing number of model runs.
- The lower/upper bounds of the main indices are wider than those of the total indices.
- The estimator of the main indices to have a larger variance than the estimator of the total indices.

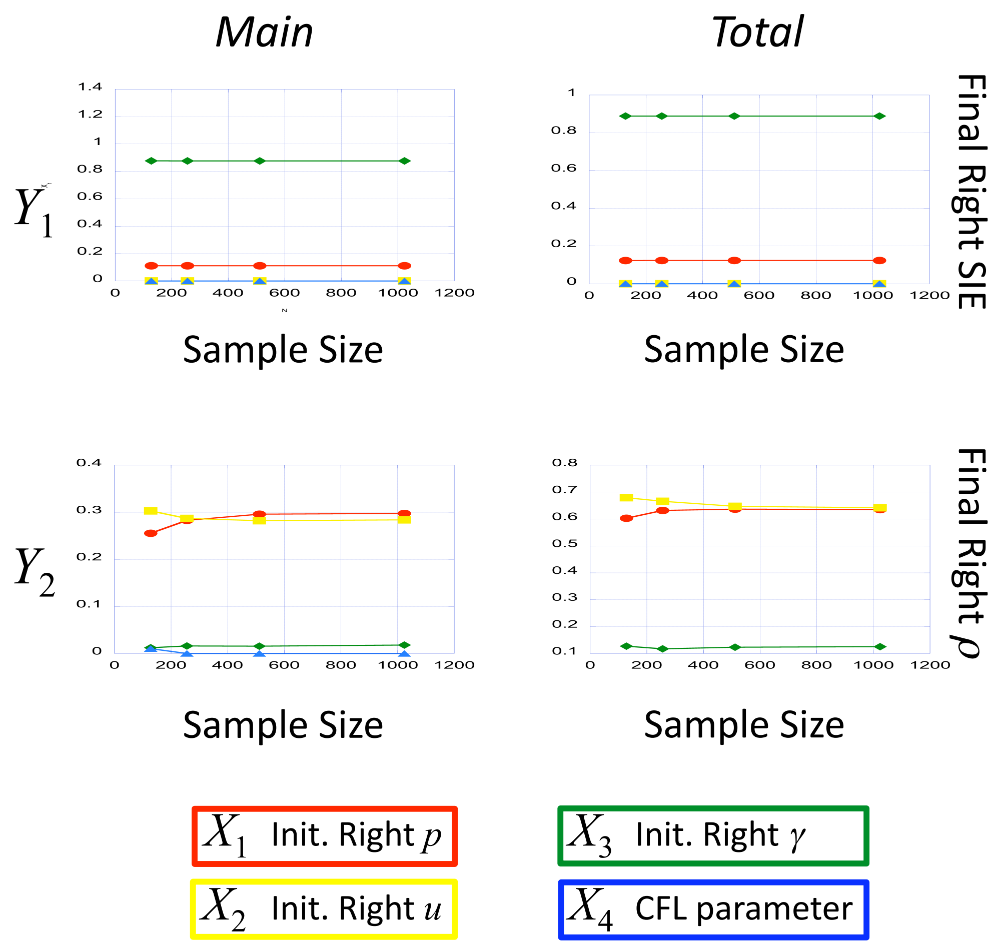


§ Saltelli, A., P. Annoni, I. Azzini, F. Campolongo, M. Ratto, S. Tarantola, "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index," *Comp. Physics Comm.*, **181**, 259–270 (2010).

* G.E.B. Archer, A. Saltelli, I.M. Sobol´, "Sensitivity Measures, ANOVA-Like Techniques and the Use of Bootstrap," *J. Statist. Comput. Simul.*, **58**, pp. 99–120 (1997).

The main and total indices for the SDP meta-model converge with sample size.

- Meta-model results are for SDP + Sobol´ estimators built with sample sizes: N=128, 256, 512, 1024.
- Sobol´ indices are calculated with the meta-model at a set of “untried” points, i.e., points not used to build the meta-model.
- Both main and total indices are well-behaved with respect to convergence.
- The indices from N=256 are robust to further refinement.



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We have some answers to our questions…

- *Do these approaches give consistent results, e.g., for rankings?*
  - In general, the different meta-models are consistent, both in ranking and magnitude, particularly for main effects (less so for total effects).

- *Do these results vary for the different outputs?*
  - "Well-behaved" outputs (e.g., Y_1 and Y_3) are quite consistent.

- *How to these results depend on the different inputs?*
  - "Well-behaved" inputs (e.g., X_1, X_2) follow the above pattern.
  - Other inputs (X_3, X_4) show more variation for SDP and ACOSSO.
  - Correct index values can be more challenging to properly calculate when there are significant interactions among the inputs (e.g., Y_2)

We have some answers to our questions…

- *Do these results "converge"?*
  - Yes (empirically): more samples $\rightarrow$ the results "settle down"
  - No: the "converged" value might differ from the *exact* value.
- *How to sampling and meta-model results compare?*
  - In general, these two methods give comparable results.
- *Can we distinguish among different meta-models?*
  - The actual numbers varied slightly, but the rankings are robust.
- *How to exact solution results compare to ALEGRA results?*
  - "Well-behaved" inputs (e.g., X_1, X_2) follow the above pattern.

- LHS 6000
- LHS 60000
- PCE4 256
- JRC 196k
- PCE6 1296
- SDP 256
- ACOSSO 256
- DACE 256

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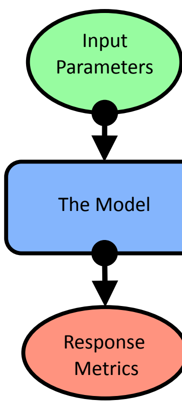
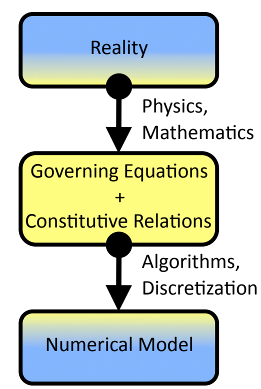
Summary: What did we talk about?

- Sensitivity Analysis :
  - Sobol'/Saltelli estimators of indices from quasi-random sampling DAKOTA
  - Sensitivity analysis using meta-models
    - PCE (DAKOTA)
    - SDP
    - ACOSSO
    - DACE (GP)



- The Application:
  - The specific problem considered—and why
  - Inputs, outputs, and what we expected
- Computer Simulations:
  - The sensitivity analysis of the simulation model does not always match that of the exact model



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Conclusions

- We considered real-physics test problem, with an exact sol'n.
- The response surfaces for computed and exact solutions were compared and exhibited discontinuous behavior.
- Monte Carlo sampling gave bounded convergence for standard sensitivity measures.
- All meta-models gave consistent main effects index values.
- Greater variability was seen for some outputs with both "small" and "large" LHS-based indices.
- Differences between the computational model and the exact model were observed.
- This study led to improvements in DAKOTA algorithms.
- We will extend this study to consider discrete inputs.

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